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PROCEDURE

EVALUATION OF DATA
FOR USABILITY IN FINAL REPORTS

RF/RMRS-98-200

Revision 0

Date Effective: 8/14/98

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APPROVED: LFPH Hughes 8/12/98
Fred Hughes, Vice President of Operations

1. PURPOSE

The purpose of this procedure is to provide a means by which a final evaluation of data quality can be performed before use in Reports generated for Environmental Monitoring and Restoration and Deactivation and Decommissioning programs and projects conducted by RMRS. Subsequent to the validation of the laboratory data, this protocol will evaluate final usability of the project data. Use of this procedure will ensure that the level of compliance with Data Quality Objectives (DQOs) is clearly communicated in Final Reports.

2. SCOPE

This procedure replaces 2-G32-ER-ADM-08.02 and applies to all RMRS employees and subcontractors who use data collected at the project level to support decision documents. This procedure is based on the relationship of data to the DQOs. Stated simply, the data are usable without qualification if project-specific DQO criteria are met; otherwise, use of data must be qualified. Within the context of this procedure, *usability* is synonymous with *adequacy* when evaluating radiochemistry data.

This procedure includes the consideration of laboratory qualifiers and codes assigned during the validation process, but is more robust and includes evaluation of all project specific DQOs. Data validation is performed by an independent, third party subcontractor to, ensure that the proper chemistry laboratory protocols are followed.

This procedure is based on requirements set forth in the RMRS Quality Assurance Program Description (QAPD) (RMRS 1998), Department of Energy (DOE) Data Management Requirements (DOE 1993) and Environmental Protection Agency (EPA) Guidelines (EPA, 1980, 1987, 1989, 1993_a, 1993_b). Specifically, precision, accuracy, representativeness, completeness, and comparability (PARCC) parameters are required based on the QAPD (RMRS 1998) and DOE Data Management Requirements (DOE, 1993). The 7-Step Process, which is the latest EPA guidance in the DQO process, is addressed in EPA 1993_a and EPA 1993_b.

ADMIN RECORD

SW-A -002700

3. DEFINITIONS AND ACRONYMS

3.1 Definitions

Accuracy. A quantitative measure of data quality, which refers to the degree of difference between, measured or calculated values and the true value of a parameter. The closer the measurement to the true value (concentration), the more accurate the measurement.

Comparability. A qualitative measure defined by the confidence with which one data set can be compared to another. Statistical tests may be used for quantitative comparison between sample sets (populations).

Completeness. A quantitative measure of data quality expressed as the percentage of valid or acceptable data obtained from a measurement system.

Data Quality Objectives (DQOs). Statements that outline the decision-making process and specify the type, quality, and quantity of data required to support decisions.

Data Validation. The process of determining adequacy and usability of the data obtained.

Field Duplicate. A field duplicate is a second sample collected at the same location as the original sample. Duplicate samples are collected simultaneously or in immediate succession, using identical recovery techniques, and treated in an identical manner during storage, transportation, and analysis, and are submitted to the laboratory as a blind sample.

Precision. A quantitative measure of data quality which refers to the reproducibility or degree of agreement among replicate measurements of a parameter. The closer the numerical values of the measurements are to each other, the lower the Relative Percent Difference.

Project Manager. A designated person responsible for scope development, budgets coordination and control, design, construction, startup and project close-out. A Project Manager has functional responsibility for all groups associated with the project and is the single point of accountability and responsibility for all events associated with the assigned projects.

Relative Percent Difference (RPD). A measure of precision, which is based upon the mean of two values from related, analyses and is reported as a

percentage. The RPD requirements are stated in the Work Plan before field sampling occurs.

Replicate. A field replicate sample, also called a split, is a single sample divided into two equal parts for analysis. The sample containers are assigned an identification number in the field such that laboratory personnel performing the analysis cannot identify them as replicate samples.

Representativeness. A qualitative characteristic of data quality defined by the degree to which the data absolutely and exactly represent the characteristics of a population. Reproducibility is accomplished by obtaining an adequate number of samples from appropriate spatial locations within the medium of interest.

Subject Matter Expert. An identified person who is knowledgeable in a specific field of interest.

Total Propagated Uncertainty. The addition of the square root of the sum of the squares of the random components of the individual uncertainties, plus the magnitude of the estimated individual systematic relative uncertainties. TPU may include uncertainties introduced through field sampling and analytical laboratory procedures.

3.2 **Acronyms**

SAP	Sampling and Analysis Plan
SWD	Soil Water Database
DOE	United States Department of Energy
DQOs	Data Quality Objectives
EPA	United State Environmental Protection Agency
ER	Environmental Restoration
Ft BGS	Feet Below Ground Surface
MDL	Method Detection Limit
µg/L	Micrograms Per Liter
PARCC	Precision, Accuracy, Representativeness, Completeness, and Comparability
PCE	Perchloroethene (tetrachloroethene)
PM	Project Manager
QAPD	Quality Assurance Program Description
RPD	Relative Percent Recovery
SME	Subject-matter Expert
SOPs	Standard Operating Procedures

TCE	Trichloroethene
TPU	Total Propagated Uncertainty
VOC	Volatile Organic Compound

4. RESPONSIBILITIES

- 4.1 **Project Manager (PM), Subject-Matter Expert (SME), or Designee**
Is responsible for the implementation of this procedure.

5. INSTRUCTIONS

NOTE: *The process described in these instructions is illustrated in Appendix 1, Process Flow for Evaluation of Data for Usability.*

PM, SME, or Designee

Ensure that a peer reviewer documents verification of the calculation addressed in this procedure on the Document Review Sheet prepared in accordance with procedure DC-06.01, Document Control Program.

5.1 **Data Validation Process**

5.1.1 **Determining Precision**

PM, SME, or Designee

- [1] For analytical data, assemble all results for field-duplicate and replicate samples and the results from the corresponding real samples.
- [2] Calculate RPD values for the sample sets (identified above) using Equation 1.

$$\text{Relative Percent Difference} = \frac{[C_1 - C_2]}{(C_1 + C_2)/2} \times 100 \quad (\text{EQUATION 1})$$

where:

C_1 = Concentration of the analyte in the real sample

C_2 = Concentration of the analyte in the duplicate/replicate

- [3] Summarize the RPD values in a tabular format with results broken out by matrix type and analytical suite

[A] Include the following in the summary:

- Calculated RPD values, and
- Overall percentages of sample sets that comply with the established precision DQO.

NOTE: *Typical RPD values for in water are $\leq 30\%$, for soil $\leq 40\%$. At least 85% of all quality control samples are required to comply with the established precision, or RPD goals.*

[B] Some examples of matrix types and analytical suites are listed in Table 1, Common Examples of Matrix Types and Analytical Suites. An example of the calculated RPD values is provided in Table 2, Calculated RPD Values. An example of the summary is provided in Table 3, Summary of RPDs.

[4] State the precision of each field or physical measurement type that ultimately influences project decisions.

Examples of field or physical measurements include the following:

- Flow rate
- Temperature
- Displacement
- Pressure
- Mass

[A] For all radiological analyses, the normalized absolute difference between the sample and the laboratory duplicate, given by the relationship below, is used in testing the null hypothesis that the results do not differ significantly when compared to their respective Total Propagated Uncertainty (TPU).

$$\frac{|S-D|}{\sqrt{TPU_s^2 + TPU_d^2}}$$

Where TPU_s = Total Propagated Uncertainty of the sample
 TPU_d = Total Propagated Uncertainty of the duplicate
S = Sample result
D = Laboratory duplicate result

- [B] If the sample or laboratory duplicate results are less than their respective Minimal Detectable Concentration (MDC), the results may still be used in this relationship to determine precision.
- [C] If the normalized absolute difference is greater than 1.96, qualify the affected sample results "J", as at the 5% level of significance, the conclusion is reached that the sample and the laboratory duplicate differ.
- [5] **IF** the calculated RPD or overall precision values for the collected samples do **NOT** fall within the accepted control limits for Precision, **THEN**:
- [A] Indicate how precision does not comply with DQO specifications.
- [B] Explain and justify the deficiencies.
- [C] Determine if additional sampling is required.

Table 1 - Common Examples of Matrix Types and Analytical Suites

<u>Matrix Type</u>	<u>Analytical Suites</u>
Air	Volatile Organic Compounds
Biota	Semi-Volatile Organic Compounds
Groundwater	Metals (inorganics)- dissolved, total
Sediment	Radionuclides - dissolved, total
Soil	Pesticides/PCBs
Surface Water	Water Quality: total, dissolved solids nitrates/nitrites other anions Field Parameters: pH temperature specific conductivity dissolved oxygen

Table 2 - Calculated RPD Values

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	Media	Detected Analyte	QC Sample Type	Associated Real Sample ID	QC Sample Result	Real Sample Result	RPD Value
QC Sample ID							
GW02479IT	Water	TCE	DUP	GW02437IT	110µg/l	100µg/l	9.5%
GW02586IT	Water	TCE	DUP	GW02440IT	84µg/l	54µg/l	43%
GW02603IT	Water	TCE	DUP	GW02601IT	250µg/l	281µg/l	11.3%

Table 3 - Summary of RPDs

Analytical Suite	Medium	Required RPD Value	Total duplicates collected	Number of duplicates within the RPD	Overall Precision Compliance
TCE	Water	≤ 30%	3	2	67% ^A
Vinyl Chloride	Soil	≤ 40%	15	13	86%

^A 2 of the 3 RPD values were within the 30% tolerance; $2/3 \times 100 = 67\%$

5.1.2 Determining Accuracy

PM, SME, or Designee

- [1] For all analytical data, compare the required analytical method and detection limit with the actual method used and its detection limit for each medium and analyte. Table 4, Comparison of Detection Limits, serve as an example for volatile organic analytes; and Required Detection Limits (RDLs) for radiochemicals are given in Kaiser-Hill Analytical Services Division Statement of Work for Analytical Measurements.

5.1.2[1] EXAMPLE - Analytical Method and Detection Limit Comparison

The Sampling and Analysis Plan (SAP) requires that method 502.2 be used for analyzing VOCs in water. For vinyl chloride, the data from the Soil and Water Database (SWD) indicate that the actual analytical method be used was not the same as the required method, and therefore, does not meet the method detection limit (MDL) requirement as identified in the laboratory statement of work. Therefore, the analytical results for vinyl chloride must be qualified as having an actual MDL of 0.18 µg/l (EPA Method 601) in contrast to the planned EPA Method 502.2 (MDL of 0.01 µg/l).

Table 4 - Comparison of Detection Limits

Analyte	Required Analytical Method	Actual Analytical Method	Required MDL ^a ug/l	Actual MDL ug/l
PCE	502.2	502.2	0.02	0.02
TCE	502.2	502.2	0.03	0.03
Vinyl Chloride	502.2	601	0.01	0.18

^a In this example, the MDL is the Required Detection Limit

[2] For field or physical measurements, state the accuracy of each instrument type that ultimately influences project decisions.

- Flow Rate
- Temperature
- Displacement
- Pressure
- Mass

NOTE: *Accuracy is based on detection limits such as from the laboratory Statement of Work specifications, manufacturer's specifications, standard operating procedures, or instrument specific calibration data. Table 5, Water Level results, serves as an example.*

[3] Evaluate the correct resolution of all reported results as well as the number of significant figures, and report all of the corresponding measurements or calculation results (for example, numerical model output) consistently.

5.1.2[3] EXAMPLE - Appropriate Resolution and Significant Figures

According to the 5-21000-OPS-GW.1, Rev. 2, water level are to be measured within 0.01 ft. The results obtained through the use of a *Solinst* Water-Level Probe, from a sampling round of water level measurements for six monitoring wells, are listed in Table 5. The data will be used for modeling the potentiometric surface of a shallow aquifer.

The data reported for MW-80 must be qualified for further use in data reduction and analysis because it does not reflect the required measurement resolution (0.01) or accuracy(0.05 ft.). Likewise, the MW-83 data must be rounded to the appropriate resolution and significant figures because it reflects measurement capabilities to 0.001 ft, which is not within the resolution of the water-level measuring device.

Table 5 - Water Level Results

Monitoring Well Number	Date Measured	Top of Water (Ft BGS)	Bottom of Well (Ft BGS)
MW-78	12/05/93	16.34	22.81
MW-79	12/05/93	18.01	24.22
MW-80	12/05/93	15.9	21.4
MW-81	12/05/93	16.02	22.69
MW-82	12/05/93	16.32	23.66
MW-83	12/05/93	17.230	25.450

- [4] **IF** any accuracy tolerance doe NOT comply with DQO specifications,
THEN:
- [A] Indicate how accuracy does not comply with DQO Specifications.
 - [B] Explain and justify the deficiencies.
 - [C] Determine if additional sampling is required.

5.1.3 Determining Representativeness

PM, SME, or Designee,

- [1] Compare the actual sample types and quantities collected with those stated in the Field Sampling Plan, per media type and analytical suite and/or per physical measurement type.

A tabular format is recommended to clearly communicate this information. An example is shown in Table 6, Sample Comparison (Required-vs-Actual).

Table 6 - Sample Comparison (Required-vs-Actual)

	Required Number of Samples per Sampling Plan Specifications	Actual Number of Samples	Deviation	Justification
Surface Soils				
Radionuclides	30	35	+5	Extra samples within budget; DOE approved
Metals	20	20		
Semi-VolatileOrganic Compounds	25	25	0	
Groundwater				
Metals	12	10	-2	Not enough sample medium to fullfill requirements
Radionuclides	12	12	0	

IF a particular analyte within an analytical suite is **NOT** or measured, **BUT** the bulk of the analytes was collected or measured, **THEN** footnote those analytes **NOT** collected and explain in the summary.

For example, "gross alpha/beta" are analytes within the radionuclide analytical suite, which may additionally contain $^{239/240}\text{Pu}$, $^{233/234,235,238}\text{U}$, tritium, $^{230/232}\text{Th}$, and ^{241}Am .

- [2] IF actual sample types and quantities do **NOT** follow associated sample controlling documents (such as the Sampling Analysis Plan), **THEN**:

- [A] Indicate how representativeness does not comply with DQO specifications.
- [B] Explained and justified deficiencies.
- [C] Determine if additional sampling is required.

5.1.4 Determining Completeness

- [1] Review analytical chemistry data with respect to matrix type and analytical suite, specifically:
 - For real samples
 - For Quality Control samples
- [2] Use equation 2 to calculate completeness for all types of data that contribute to project decisions, including the following:
 - Water-level measurements
 - Periodic flowrates
 - Temperatures

$$\text{Completeness} = DP_u = \frac{DP_t - DP_n}{DP_t} \times 100\% \quad (\text{EQUATION 2})$$

Where:

DP_u = Percentage of usable data points

DP_n = non usable data points

DP_t = Total number of data points

Example:

x = usable VOC soil samples

y = 8 non usable VOC soil samples

t = 46 total number of VOC soil samples collected

$$\text{Completeness: } x = \frac{46 - 8}{46} \times 100\%$$

$$x = 83\%$$

Without 90% as a goal, $DP_u < 90\%$. Therefore, the soil sampling program is considered to be incomplete and additional VOC samples may be required to full fill the Sampling and Analysis Plan.

- [3] **IF** actual sample types and quantities do **NOT** follow associated sample-controlling documents (such as the Sampling and Analysis Plan), **THEN**:
- [A] Indicate how completeness does not comply with DQO specifications
 - [B] Explain and justify deficiencies
 - [C] Determine if additional sampling is required.

5.1.5 Determining Comparability for Analytical Chemistry and Radionuclide Data PM, SME, or Designee,

- [1] Demonstrate comparability of data sets with respect to one or more of the following commonalties:

Protocols (e.g., SOPs) used to collect or synthesize the samples

- Matrix types (such as soil vs. Water)
- Temporal considerations (periodical, seasonal, event-related)
- Spatial considerations (3-dimensional)

NOTE: *Comparability is required to include at a minimum the comparison of real samples with other real samples, as appropriate.*

- [2] **IF** actual sample types and quantities do **NOT** follow associated sample-controlling documents (such as the Sampling and Analysis Plan), **THEN**:
- [A] Indicate how comparability does not comply with DQO specifications
 - [B] Explain and justify deficiencies
 - [C] Determine if additional sampling is required.

5.1.6 Comparison of Environmental Samples with Blanks (Quality Control Samples) PM, SME, or Designee

- [1] **WHEN** completing this section,
THEN consider all quality control QC samples collected during the field project, except duplicates and replicates, including the following :

-
- Trip blanks
 - Rinsates
 - Preservation blanks
 - Any other field blanks.
- [2] **IF** a detected analyte is a common laboratory contaminant
AND the real sample concentration is less than 10 times the blank concentration,
THEN conclude that the potential contaminant of concern is a laboratory contaminant in the real sample.
- [3] **IF** a detected analyte is a common laboratory contaminant,
AND the real sample concentration is greater than or equal to 10 times the blank concentration,
THEN conclude that the analyte in the real sample is a true detect. (US EPA, 1989)
- [4] **IF** a detected analyte is **NOT** a common laboratory contaminant,
AND the real sample concentration is less than 5 times the blank concentration,
THEN conclude that the analyte in the real sample is a true detect (US EPA, 1989).
- [5] **IF** a detected analyte is **NOT** a common laboratory contaminant,
AND the real sample concentration is greater than or equal to 5 times the blank concentration,
THEN conclude that the analyte in the real sample is a true detect (US EPA, 1989)
- [6] **IF** the source of detected contamination from real or QC samples is inconclusive,
THEN compare lot of numbers of sampling containers used for real samples with analytical results for the same lots of sample containers produced by the laboratory.
- This process should determine if the sample containers are the source of contamination.
- [7] Summarize the QC sample data by listing in tabular format the parameters listed in Table 7, QC Sample Summary, with respect to matrix type and analytical suite.

Table 7 - QC Sample Summary

	QC Sample Type	QC Sample Date Collected	Assoc. Real Sample ID	Real Sample Date Collected	QC Sample Result	Real Sample Result	Units	Detect in Blank (yes/no)
QC Sample ID								
QC Sample ID								
QC Sample ID								

This Table is an example of format only.

5.2 The Seven Step DQO Process (EPA, 1993)

PM, SME, or Designee

- [1] **IF** the Seven-Step DQO process was initiated at the project's beginning,
THEN compare report conclusions with the decisions and decision error
tolerances stipulated by the project.
- [2] Explain and justify any discrepancies between the DQOs and inadequacies of
information and conclusions stated in the report.

6. RECORDS

There are no quality or non quality records generated by this procedure.

7. REFERENCES

DOE, 1993, Data Management Requirements; Section 5, Management Procedures and Requirements; U.S. Department of Energy Rocky Flats Plant Environmental Restoration.

EPA, 1993, Guidance for Planning for Data Collection in Support of Environmental Decision Making Using the Data Quality Objectives Process, Interim Final; Office of Research and Development, Washington D.C.; EPA QA/G-4.

EPA, 1993, Data Quality Objectives Process for SUPERFUND: Interim Final Guidance; Office of Solid Waste and Emergency Response, Washington D.C.; EPA 540-R-93-071.

EPA, 1989, Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part A); Office of Emergency and Remedial Response, Washington D.C.; EPA/540/1-89/002.

EPA, 1987, Data Quality Objectives for Remedial Response Activities, Development Process; Office of Emergency and Remedial Response, Washington D.C.; EPA/540/G-87/003.

EPA, 1980, Interim Guidelines and Specifications for Preparing Quality Assurance Project Plans, QAMS-005/80, Washington, DC.

RMRS, 1998, Wide Quality Assurance Program Description, Rocky Flats Environmental Technology Site, Golden, CO.

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